

Journal of Magnetic Resonance

EDITOR: Wallace S. Brey, Jr.

EDITORIAL BOARD:

E. Raymond Andrew
Edwin D. Becker
James W. Cooper
B. P. Dailey
P. Diehl
Richard Ernst
Ray Freeman
J. H. Goldstein

David M. Grant
R. K. Harris
K. H. Hausser
Charles S. Johnson, Jr.
J. Jonas
Lowell Kispert
Masaji Kubo
George C. Levy

Ralph Livingston
Bruce McGarvey
Rex E. Richards
Max T. Rogers
Ian C. P. Smith
J. B. Stothers
Robert L. Vold

Volume 37, 1980



ACADEMIC PRESS
New York and London

A Subsidiary of Harcourt Brace Jovanovich, Publishers

Copyright © 1980 by Academic Press, Inc.

All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (Operations Staff, P.O. Box 765, Schenectady, New York 12301), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1980 articles are the same as those shown for current articles.

Made in Great Britain

CONTENTS OF VOLUME 37

NUMBER 1, JANUARY 15, 1980

M. A. HEMMINGA AND P. A. DE JAGER. The Study of Flow by Pulsed Nuclear Magnetic Resonance. II. Measurement of Flow Velocities Using a Repetitive Pulse Method	1
SHIGENOBU HAYASHI, KIKUKO HAYAMIZU, AND OSAMU YAMAMOTO. Spin-Spin Coupling Constants between Carbon-13 and Bromine and Their Correlation with the <i>s</i> Character of the Carbon Hybridization	17
STEPHEN P. DOHERTY. A Simple and Inexpensive Pulsed NMR Data Acquisition System	31
B. SCHNEIDER, D. DOSKOČILOVÁ, J. BABKA, AND Z. RŮŽIČKA. A Variable-Temperature Probe for the Measurement of ¹ H NMR Spectra with Magic-Angle Rotation	41
ROBERT G. C. McELROY, JAMES Y. HWANG, AND ROBIN L. ARMSTRONG. Temperature Dependence of the ¹²⁷ I Nuclear Quadrupole Resonance Frequency in (NH ₄) ₂ PtI ₆	49
N. KLIMES, G. LASSMANN, AND B. EBERT. Time-Resolved EPR Spectroscopy. Stopped-Flow EPR Apparatus for Biological Application	53
P. S. ALBRAND, E. W. RANDALL, AND R. M. LYNDEN-BELL. Transient Oscillations in Heteronuclear Double Resonance Spectra of Coupled Systems	61
R. F. KARLICEK, JR, AND I. J. LOWE. A Modified Pulsed Gradient Technique for Measuring Diffusion in the Presence of Large Background Gradients	75
G. BODENHAUSEN, R. L. VOLD, AND R. R. VOLD. Multiple Quantum Spin-Echo Spectroscopy	93
A. J. VEGA, A. D. ENGLISH, AND W. MAHLER. Chemical-Shift Relaxation in Multiple-Pulse NMR	107
J. A. BURT. Experimental and Theoretical Analysis of Spurious EPR Line Features Caused by Field Inhomogeneity	129
R. CASSELS, C. M. DOBSON, F. M. POULSEN, R. G. RATCLIFFE, AND R. J. P. WILLIAMS. Transverse Relaxation Effects Resulting from Deuterium Exchange in the Proton NMR Spectra of Proteins	141

COMMUNICATIONS

JOSEPH E. SARNESKI, LUTHER E. ERICKSON, AND CHARLES N. REILLEY. Additive Multipath Coupling between Platinum and Carbon in the Framework of Small Ring systems	155
D. ALLAN BUTTERFIELD AND MICHAEL A. FITZPATRICK. Electron Paramagnetic Resonance Investigations of the Effects of Diethylstilbestrol on the Physical State of Membrane Lipids and Proteins	159
S. J. OPELLA, M. H. FREY, AND J. A. DiVERDI. Quick Sample Change Probe for Magic-Angle-Spinning NMR in a Superconducting Magnet	165
S. J. OPELLA AND T. A. CROSS. Enhanced Selection of Nonprotonated Carbon Resonances in Solution NMR	171
AD BAX AND RAY FREEMAN. Enhanced NMR Resolution by Restricting the Effective Sample Volume	177

NUMBER 2, JANUARY 30, 1979

ULF EDLUND AND SVANTE WOLD. Interpretation of NMR Substituent Parameters by the Use of a Pattern Recognition Approach	183
D. VAN ORMONDT, K. V. REDDY, M. A. VAN AST, H. W. DEN HARTOG, AND E. J. BIJVANK. ENDOR of Gadolinium Ion in SrCl_2 : A Study of the Hyperfine Interaction	195
WILLIAM H. NELSON. Quick-Access Sample System for Low-Temperature ESR/ENDOR at <i>K</i> -Band	205
ALEX D. BAIN. Superspin in NMR: Application to the ABX System	209
K. M. MORE, G. R. EATON, AND S. S. EATON. Magnetic Susceptibility and EPR Changes Caused by Grinding of Samples	217
KARL-AKE THUOMAS, ANDERS ERIKSSON, AND ANDERS LUND. An Analysis of the Influence of Zero-Point Vibrations on Magnetic Hyperfine Interactions in $\cdot\text{NH}_2$, $\cdot\text{NH}_3^+$, and $\cdot\text{N}_2\text{H}_4^+$	223
VIVIAN S. F. CHEW AND JAMES R. BOLTON. The Analysis of the EPR Spectrum of the 10-Hydro-5-methyl-Ohenazinium Cation Radical	231
P. DE GROOT AND P. VAN HECKE. Selective Pulse NMR Experiments in Solid Organic Free Radicals	241
P. T. CALLAGHAN, C. M. TROTTER, AND K. W. JOLLEY. A Pulsed Field Gradient System for a Fourier Transform Spectrometer	247

O. LUTZ AND H. OEHLER. ^{138}La and ^{139}La Nuclear Magnetic Resonance Studies	261
T. J. BASTOW AND H. J. WHITFIELD. NQR in Metal Dihalides MX_2 . . .	269
G. FRONZA, R. MONDELLI, F. LELJ, E. W. RANDALL, AND C. A. VERACINI. Structural Changes Induced in the NH_2 Group of Aniline by Substituents: The Structure and Orientation of para-Bromo- and para-Nitroaniline [$1\text{-}^{15}\text{N}$] in Nematic Liquid Crystal Solvents by NMR . .	275
T. C. WONG AND LAWRENCE J. ALTMAN. Tritium and Proton Nuclear Magnetic Resonance Study of the Isotope Effects on the Molecular Structure and the Degree of Order of Partially Oriented [$^3\text{H}_1$]Benzen .	285
F. GEOFFREY HERRING, ALAN G. MARSHALL, PAUL S. PHILLIPS, AND D. CHRISTOPHER ROE. Dispersion versus Absorption (DISPA): Modulation Broadening and Instrumental Distortions in Electron Paramagnetic Resonance Lineshapes	293
R. P. J. MERKS AND R. DE BEER. Fourier Transform of the ^{133}Cs Modulation of the Electron Spin-echo Envelope of $\text{Cs}_2\text{ZnCl}_4\text{:Cu}^{2+}$	305
J. R. MORTON, K. F. PRESTON, AND S. J. STRACH. EPR Spectra in Gamma-Irradiated KPF_6 and KAsF_6	321
J. -P. KORB AND J. MARUANI. Measurement of Spin-Lattice Relaxation Rates for Inhomogeneously Broadened Lines. I. Rapid Spectral Diffusion Case	331

COMMUNICATIONS

C. L. KHETRAPAL, ANIL KUMAR, A. C. KUNWAR, P. C. MATHIAS, AND K. V. RAMANATHAN. Dimensional NMR Spectra of Oriented Molecules.	349
GEORGE C. LEVY, J. TERRY BAILEY, AND DAVID A. WRIGHT. A Sensitive NMR Thermometer for MultiNuclei FT NMR	353
MICHA POLAK, ALBERT J. HIGHE AND ROBERT W. VAUGHAN. Enhanced Resolution in NMR of Quadrupolar Nuclei in Solids: Interferometric Correlation of the First- and Second-Order Shifts .	357
F. DEBRECZENI AND I. NAGYPAL. Calculation of Paramagnetic Contribution to NMR Linewidth	363
J. P. JACOBSEN. Assignment of Relative Signs of Dipole-Dipole Couplings in Nematic Phase by Use of Selective Spin Population transfer (SPT)	365

GEORGE H. WEISS, RAJ K. GUPTA, JAMES A. FERRETTI, AND EDWIN D. BECKER. The Choice of Optimal parameters for Measurement of Spin-Lattice Relaxation Times. I. Mathematical Formulation	369
EDWIN D. BECKER, JAMES A. FERRETTI, RAJ K. GUPTA, AND GEORGE H. WEISS. The Choice of Optimal Parameters for Measurement of Spin-Lattice Relaxation Times. II. Comparison of Saturation Recovery, Inversion, Recovery, and Fast Inversion Recovery Experiments	381
DAVID S. STEPHENSON AND GERHARD BINSCH. Automated Analysis of High-Resolution NMR Spectra. I. Principles and Computational Strategy	395
DAVID S. STEPHENSON AND GERHARD BINSCH. Automated Analysis of High-Resolution NMR Spectra. II. Illustrative Applications of the Computer Program DAVINS	409
F. RIBAS PRADO, C. GIESSNER-PRETTRE, J-P. DAUDEY, A. PULLMAN, J. F. HINTON, G. YOUNG, AND D. HARPOOL. Nuclear Magnetic Resonance Spectroscopy Applied to Li^+ Complexation by Small Ligands: An <i>ab Initio</i> and Experimental Study of ^7Li Chemical Shifts	431
JIMMY H. DAVIS, HSIANG-NING SUN, DAVID REDFIELD, AND GALEN D. STUCKY. The Proton and Carbon NMR Spectra of Alkyl-Substituted Titanocene and Zirconocene Dichlorides	441
YONA SIDERER AND ZEEV LUZ. Analytical Expressions for Magnetic Resonance Lineshapes of Powder Samples	449
KENNETH R. JEFFREY. Phase-Splitting Circuits for Use in a Pulsed NMR Spectrometer	465
L. S. BATCHELDER AND J. L. RAGLE. Nitrogen Quadrupole Coupling in Paraelectric Ammonium Sulfate	469
M. MEHRING, E. K. WOLFF, AND M. E. STOLL. Exploration of the Eight-Dimensional Spin Space of a Spin-1 Particle by NMR	475
ROBERT D. ALLENDOERFER AND JAMES B. CARROLL, JR. A Coaxial Microwave Cavity for Improved Electron Paramagnetic Resonance Sensitivity with Lossy Solvents	497
S. EMID, J. KONIJNENDIJK, AND J. SMIDT. Measurement of Short Dipolar Relaxation Times by the Saturation Method	509
J. LABSKÝ, J. PILAŘ, AND J. LÖVY. Magnetic Resonance Study of 4-Amino-2,2,6,6-tetramethylpiperidine- <i>N</i> -oxyl and Its Deuterated Derivatives	515
RICHARD W. BRIGGS, FELICIA A. ETZKORN, AND JAMES F. HINTON. ^{205}Tl Nuclear Magnetic Resonance Study of the Thallium Complex of Lasalocid (X-537A)	523

W. M. SHIRLEY AND Z. Z. HUGUS, JR. The Temperature Dependences of Halogen and Cobalt NQR Frequencies in <i>trans</i> -Dichlorobis(ethylenediamine)cobalt(III) Chloride Hydrochloride Dihydrate and Related Compounds	529
--	-----

COMMUNICATIONS

D. L. WEAVER. Diffusion and the "Fast-Exchange" Model	543
JAMES L. ENGLE. Low-Noise Broadband Transmit/Receive Circuit for NMR	547
ANDREAS SCHWENK. Comment on the Communication, " ⁸⁹ Y Spin-Spin Relaxation Times are Not pH Dependent"	551
R. D. KENDRICK, C. S. YANNONI, R. AIKMAN, AND R. J. LAGOW. Scalar Coupling between Rare Spins in Solids	555
AUTHOR INDEX FOR VOLUME 37	557

The Subject Index for Volume 37 will appear in the December 1980 issue as part of a cumulative index for the year 1980.



Digitized by the Internet Archive
in 2023

Information for Authors

The *Journal of Magnetic Resonance* includes original papers, both full articles and communications, dealing with the theory, techniques, methods of spectral analysis and interpretation, spectral correlations and results of magnetic resonance spectroscopy and related fields. The Editor seeks the assistance of expert referees in the evaluation of manuscripts of articles, but he alone is responsible for the final decision concerning acceptance.

Original papers only will be considered. Manuscripts are accepted for review with the understanding that the same work has not been and will not be published nor is presently submitted elsewhere, and that all persons listed as authors have given their approval for the submission of the paper; further, that any person cited as a source of personal communications has approved such citation. Written authorization may be required at the Editor's discretion. Articles and any other material published in the *Journal of Magnetic Resonance* represent the opinions of the author(s) and should not be construed to reflect the opinions of the Editor(s) and the Publisher.

Authors submitting a manuscript do so on the understanding that if it is accepted for publication, copyright in the article, including the right to reproduce the article in all forms and media, shall be assigned exclusively to the Publisher. The Publisher will not refuse any reasonable request by the author for permission to reproduce any of his or her contributions to the journal.

Communications are preliminary accounts of work of special importance or contain discussion of controversial subjects. Communications must be especially carefully and concisely prepared; since they may not be refereed, it is the responsibility of the author to ensure that the manuscript as originally submitted is free of typographical or substantive errors.

Fifty reprints of each paper are supplied without charge, and additional reprints may be ordered on a form which is sent to the authors along with the galley proofs which the author receives. The Journal assesses no page or publication charges.

All manuscripts and books for review should be sent to the editor, Wallace S. Brey, Department of Chemistry, University of Florida, Gainesville, Florida 32611.

Arrangement of the Paper

If the paper is lengthy, it should be divided into sections, although it is preferred that the sections not be numbered. Tables are numbered consecutively with *Arabic* numerals and are to be mentioned in order in the text. Each table should be supplied with a title. Figures are also numbered consecutively with *Arabic* numerals and are mentioned in order in the text. Each regular article requires an abstract which should describe concisely the substantive content, the conclusions reached, and the contributions of the research described. Since the abstract may be used directly by Chemical Abstracts and other abstracting services, it must be self-contained, having no references to formulas, equations, or bibliographic citations which appear in the body of the manuscript.

Literature references are cited in numerical order in the text by *in-line, parenthesized, italic numerals*. References to "unpublished" or "to be published" work from the author's laboratory should not be given. However, dissertations may be cited, or papers actually accepted may be referred to as "in press" if the name of the journal is included.

Authors are urged to give careful thought to the logical construction of the manuscript, so that explanatory or parenthetical footnotes need not be employed. Any footnotes which are indispensable are not intermixed with references, but are indicated in the text by consecutive, superscript numerals, and each footnote will then appear in the print at the bottom of the page on which it is cited. Equation numbers are given in *square* brackets to the right of the equation, and references in the text to equations should be in the form "Eq. [3]."

Form of Manuscript

Manuscripts should be submitted in triplicate. The *original typewritten copy* should be supplied; mimeo, electrostatic and similar process reproductions are not usually sufficiently clear. All of the typing must be

double-spaced, including that of abstract, references, and footnotes, on one side of good quality paper approximately 22 × 28 cm (8.5 × 11 in.) in dimensions. The first line of each paragraph is indented.

Each page of the manuscript should be numbered. The first page contains the article title, the author's name, and affiliation. At the bottom of this page should appear any footnotes to the title (indicated by superscript *, †, ‡); the number of manuscript pages, figures, and tables should also be noted. The second page should contain the abstract of 50–200 words.

Symbols and Abbreviations. The American Chemical Society's Handbook for Authors, 1978 edition or the Style Manual of the American Institute of Physics should be followed for standard abbreviations, names and symbols for units. Mathematical equations or symbols must be typewritten whenever possible. Greek letters may be identified in pencil in the margin. The author of any manuscript in which there are mathematical symbols is urged to supply a list identifying the characters required for the assistance of the printer in selecting the proper type. The list will not appear in print.

References and Footnotes. References to the literature should be cited in order in the text by in-line, parenthesized numerals. The references themselves are to be typed double-spaced on a separate sheet in numerical order. Each reference contains the author's initials, last name, journal name, volume, initial page number and year in parentheses, *in that order*. The name of the journal is abbreviated in the style of Chemical Abstracts Service *Source Index* (1975 Edition). For book references, the form is author's name, name of the book in quotation marks, editor's name (if any), edition if other than the first, chapter or page number, publisher's name, place of publication, and year of publication.

Any footnotes which are included are numbered in a sequence separate from the references and must be typed in the manuscript on a separate page.

Tables. Tables should be laid out carefully, so that minimum space is used and entries are accurately grouped and clearly labeled. Usually, a table should be arranged vertically, with more rows than columns. Vertical lines are not used to separate the columns. Each table is numbered with an Arabic numeral, provided with a title, and typed on a separate sheet of paper. Footnotes to the table are placed directly below it and are indicated by superscript, lower case, italic letters (^{a,b,c}). Tables that are longer than two manuscript pages will be reproduced photographically, and should therefore be typed in the exact form desired. All such tables should be carefully checked since errors cannot be corrected in proof.

Figures. Figures must be carefully drawn in black, waterproof drawing ink, to draftsman's standards, with lettering by stencil or drawing machine. Freehand, penciled, or typewritten lettering is not acceptable. Lettering should include numerical scales and units required for the two axes, and should be large enough to be legible after reduction by 50–60%. The illustration copy should be on sheets of the same size as that on which the manuscript is typed. Smaller figures may be mounted on sheets of the required size, and larger originals may be handled by supplying glossy, high-contrast, photographic reductions. The original and two duplicates of each figure are required.

Diagrams. Ink drawings should be supplied for any complex molecular formulas or diagrams involving material which the printer cannot readily set in type.